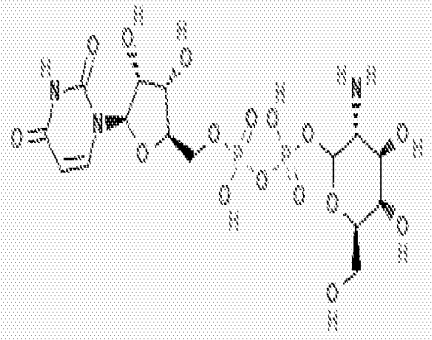
Udp galactosamine - Substance Summary (SID: 11533454)

isolated from Bacillus megaterium; intermediate in the biosynthesis of galactosamine-6-phosphate polymer

Table of Contents
- Drug and Chemical Info
- Data Source
- Synonyms
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- Descriptors
- Substance Info
- Exports

Compound Displayed: PubChem



Drug and Chemical Info from MeSH: (Total: 1)

uridine diphosphate galactosamine

PubMed

PubMed MeSH Keyword Summary

Compound ID	6857449
Molecular Weight	565.317022 [g/mol]
Molecular Formula	$C_{15}H_{25}N_3O_{16}P_2$
XLogP	-6.6
H-Bond Donor	9
H-Bond Acceptor	17

Data Source:

Depositor: ChEBI
External ID: CHEBI:22099

Links

Chemical Structure Search

Depositor-Supplied Synonyms: (Total: 8)

Sort: Weight

Udp galactosamine
UDP-D-galactosamine
Uridine diphosphate galactosamine

CHEBI:22099
Uridine 5'-diphosphogalactosamine
uridine 5'-[3-(2-amino-2-deoxy-D-galactopyranosyl) dihydrogen diphosphate]
Uridine 5'-(trihydrogen diphosphate), P'-(2-amino-2-deoxy-alpha-D-galactopyranosyl) ester
17479-06-0

Properties Computed from Structure:

Molecular Weight	565.317022 [g/mol]
Molecular Formula	$C_{15}H_{25}N_3O_{16}P_2$
XLogP	-6.6
H-Bond Donor	9
H-Bond Acceptor	17
Rotatable Bond Count	9
Tautomer Count	3
Exact Mass	565.071005
Monoisotopic Mass	565.071005
Topological Polar Surface Area	297
Heavy Atom Count	36
Formal Charge	0
Complexity	967
Isotope Atom Count	0
Defined Atom StereoCenter Count	8
Undefined Atom StereoCenter Count	1
Defined Bond StereoCenter Count	0
Undefined Bond StereoCenter Count	0
Covalently-Bonded Unit Count	1

Descriptors Computed from Structure:

IUPAC Name: [(3R,4R,5R,6R)-3-amino-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl] [[(2R,3S,4R,5R)-5-(2,4-dioxopyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy-hydroxyphosphoryl] hydrogen phosphate
Canonical SMILES: C1=CN(C(=O)NC1=O)C2C(C(C(O2)COP(=O)(O)OP(=O)(O)OC3C(C(C(C(O3)CO)O)O)N)O)O
Isomeric SMILES: C1=CN(C(=O)NC1=O)[C@H]2[C@@H]([C@@H]([C@H](O2)COP(=O)(O)OP(=O)(O)OC3[C@@H]([C@H]([C@H](O3)CO)O)O)N)O)O
InChI: InChI=1/C15H25N3O16P2/c16-8-11(23)9(21)5(3-19)32-14(8)33-36(28,29)34-35

(26,27)30-4-6-10(22)12(24)13(31-6)18-2-1-7(20)17-15(18)25/h1-2,5-6,8-14,19,21-24H,3-4,16H2,(H,26,27)(H,28,29)(H,17,20,25)/t5-,6-,8-,9+,10-,11-,12-,13-,14?/m1/s1/f/h17,26,28H

Substance Info:

SID: 11533454

Deposit Date: 2006-06-21

Modify Date: 2008-01-31

CID: 6857449

Create Date: 2006-06-21

Related Substances:

Same: 2 Links

Same, Connectivity: 17 Links

Similar Substances: 923 Links

ASN1	Display	XML	Display	SDF	Display
	Save		Save		Save